

Isopropanol-1,1,1,3,3,3-d6
3976-29-2 | DTXSID90480716

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 3.68

Global applicability domain: Inside

Local applicability domain index: 9.38e-01

Confidence level: 6.92e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Isopropanol</div> <div>Measured: 3.41</div> <div>Predicted: 3.68</div>	<div>Image not found</div> <div>Acetic acid</div> <div>Measured: 4.31</div> <div>Predicted: 3.69</div>	<div>Image not found</div> <div>1-Propanol</div> <div>Measured: 3.71</div> <div>Predicted: 3.75</div>
<div>Image not found</div> <div>Ethanol</div> <div>Measured: 3.25</div> <div>Predicted: 3.05</div>	<div>Image not found</div> <div>tert-Butyl alcohol</div> <div>Measured: 3.50</div> <div>Predicted: 3.81</div>	